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Some remarks on the calculation of the cohesive energy of ionic crystals

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This paper is a complement to the earlier quantum mechanical treatments of ionic crystals in the Heitler-London approximation, which have been given by Hylleraas, Landshoff and Löwdin. The method, which is restricted to crystals consisting of ions with complete electron shells, was founded by Hylleraas[1] in his investigation of LiH. He formulated the appropriate physical assumptions, the description of the crystal by a wave function having the correct symmetry properties and the method of subtracting the energy of the free ions. Landshoff[2] has treated NaCl by using approximately ortho-normalized one-electron wave functions obtained as linear combinations of the one-electron orbitals for the free ions. He introduced the overlap integrals $S_{\mu\nu}$ defined by formula (2) below and ortho-normalized the wave functions correctly to the first order in the $S_{\mu\nu}$, taking also certain second order terms into account. Later Löwdin[3] has used a mathematically exact method for ortho-normalizing by means of the matrix calculus. However, in his calculations he used a series expansion in the $S_{\mu\nu}$ and considered an approximation similar to Landshoff's, taking into account some further terms. Applying Löwdin's formula for the cohesive energy without introducing this expansion, we shall show how the calculations can be performed even in those cases where the series expansion mentioned is not convergent. In this connection we have found it necessary to investigate the energy expression further.

From the normalized wave functions ψ_μ associated with the free ions, a set of ortho-normalized functions φ_μ is obtained, according to Löwdin, by

$$\varphi_\mu = \sum_\alpha \psi_\alpha \{(\mathbf{1} + \boldsymbol{S})^{-\frac{1}{2}}\}_{\alpha\mu}. \tag{1}$$

The ψ_μ and φ_μ are one-electron wave functions that depend on both space coordinates, $\boldsymbol{r} = (x, y, z)$, and spin coordinate, ζ. The transformation (1) is uniquely determined except for an arbitrary unitary transformation. $\boldsymbol{S}$ is the following Hermitian matrix introduced in this problem by Landshoff:

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[1] E. A. Hylleraas, Z. f. Phys. 63, 771 (1930).

[2] R. Landshoff, Z. f. Phys. 102, 201 (1936); Phys. Rev. 52, 246 (1937).

[3] P. O. Löwdin, Dissertation, Uppsala 1948, Cf. also Arkiv f. mat., astr. o. fysik 35 A, N:o 9 and N:o 30; J. Chem. Phys. 18, 365 (1950).

$$S_{\mu\nu} = \int \psi_\mu^*(1)\, \psi_\nu(1)\, d\tau_1 - \delta_{\mu\nu} \tag{2}$$

the sign $\int d\tau_1 \cdots$ implying summation over the spin coordinate and integration over the space coordinates.[1] LÖWDIN has supposed that the symbol $(\mathbf{1} + \boldsymbol{S})^{-\frac{1}{2}}$ has a meaning. It should be remarked that for this to be true it is necessary and sufficient that $\det(\mathbf{1} + \boldsymbol{S}) \neq 0$. We shall suppose this condition to be fulfilled. In terms of the functions φ_μ the energy is given by a well-known expression. Substituting (1) into this expression, subtracting the energy of the free ions and using the fact that the ψ_μ satisfy Hartree-Fock equations, Löwdin finds the following formula for the cohesive energy[2]:

$$E_{\text{coh}} = E_1 + E_2 + E_3 + E_4, \tag{3}$$

where

$$E_1 = \frac{e^2}{2} \sum_g \sum_{g'}{}^{(g)} \frac{Z_g Z_{g'}}{r_{gg'}} + \sum_\mu (\mu \,|\, H^{(\mu)} \,|\, \mu) + \sum_\mu \sum_\nu{}^{(\mu)} (\mu\nu \,|\, G \,|\, \mu\nu) \tag{3 a}$$

$$E_2 = -\sum_\mu \sum_\nu{}^{(\mu)} (\mu\nu \,|\, G \,|\, \nu\mu) \tag{3 b}$$

$$E_3 = -\sum_\mu \sum_\nu P_{\mu\nu} \Big\{ (\nu \,|\, H^{(\mu)} \,|\, \mu) + 2 \sum_\varkappa{}^{(\mu)} \left[(\nu\varkappa \,|\, G \,|\, \mu\varkappa) - (\nu\varkappa \,|\, G \,|\, \varkappa\mu) \right] \Big\} \tag{3 c}$$

$$E_4 = \sum_\mu \sum_\nu \sum_\varkappa \sum_\lambda P_{\mu\varkappa} P_{\nu\lambda} \left\{ (\varkappa\lambda \,|\, G \,|\, \mu\nu) - (\varkappa\lambda \,|\, G \,|\, \nu\mu) \right\} \cdot \tag{3 d}$$

The new symbols here have the following meaning:

$$(\mu \,|\, H^{(\mu)} \,|\, \nu) = \int \psi_\mu^*(1) \left(-e^2 \sum_g{}^{(\mu)} \frac{Z_g}{|\boldsymbol{r}_1 - \boldsymbol{r}_g|} \right) \psi_\nu(1)\, d\tau_1$$

$$(\mu\nu | G | \varkappa\lambda) = \int\int \psi_\mu^*(1)\, \psi_\nu^*(2) \frac{e^2}{2|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \psi_\varkappa(1)\, \psi_\lambda(2)\, d\tau_1\, d\tau_2,$$

where Z_g is the charge of the nucleus g, and e is the electron charge. $\sum_\nu^{(\mu)}$ denotes a summation over all indices ν except those associated with the ion with which μ is associated.[3] The meaning of $\sum_g^{(\mu)}$ as well as $\sum_{g'}^{(g)}$ (used later) is quite analogous. The quantities $P_{\mu\nu}$ are the elements of a matrix $\boldsymbol{P}$ defined by

$$\boldsymbol{P} = \frac{\boldsymbol{S}}{\mathbf{1} + \boldsymbol{S}} \cdot \tag{4}$$

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[1] The symbol 1 in $\psi_\mu(1)$ is written as an abbreviation for the position vector $\boldsymbol{r}_1$ and the spin coordinate ζ_1 of an electron.

[2] We have written E_1, E_2 and $E_3 + E_4$ instead of Löwdin's E_{elstat}, E_{exch} and E_{S} in order to indicate clearly that it is only the sum $E_{\text{coh}} = E_1 + E_2 + E_3 + E_4$ that has a real physical interpretation.

[3] We find the notation $\sum_\nu^{(\mu)}$ simpler than that introduced by Landshoff and taken over by Löwdin.

For the sake of simplicity we now specialize the treatment to LiH. This specialization is not essential, but is made only to get somewhat simplified formulæ. The symbol μ has now reference to a definite lattice point g and a definite spin state j. We indicate this by writing $\mu = (g, j)$, $\nu = (g', j')$ and so on. The given one-electron wave functions are written

$$\psi_\mu(1) = \psi_\mu(\boldsymbol{r}_1, \zeta_1) = \psi_g(\boldsymbol{r}_1)\, \delta_{j\,\zeta_1}. \tag{5}$$

The quantities

$$s_{g g'} = \int \psi_g^*(\boldsymbol{r})\, \psi_{g'}(\boldsymbol{r})\, d\,\boldsymbol{r} - \delta_{g g'}$$

form a matrix called $\boldsymbol{s}$, the diagonal elements of which are evidently 0. We now define a new matrix $\boldsymbol{p}$ by

$$\boldsymbol{p} = \frac{\boldsymbol{s}}{\boldsymbol{1} + \boldsymbol{s}}, \tag{6}$$

which is possible if det $(\boldsymbol{1} + \boldsymbol{s}) \neq 0$. (Note that det $(\boldsymbol{1} + \boldsymbol{S}) = (\text{det } (\boldsymbol{1} + \boldsymbol{s}))^2$.) The ψ_g being real for LiH, the matrices $\boldsymbol{s}$ and $\boldsymbol{p}$ are both symmetrical. The matrices $\boldsymbol{S}$ and $\boldsymbol{P}$ are obtained by the formulæ

$$S_{\mu\nu} = s_{g g'}\, \delta_{j j'} \tag{7}$$

$$P_{\mu\nu} = p_{g g'}\, \delta_{j j'}, \tag{8}$$

where $\mu = (g, j)$ and $\nu = (g', j')$. Using (3), (3 a, b, c, d), (5) and (8), we find after some simplification the following expression for the cohesive energy of a LiH crystal[1]:

$$E_{\text{coh}} = E_1 + E_2 + E_3 + E_4, \tag{9}$$

where

$$E_1 = e^2 \sum_g \sum_{g'}{}^{(g)} \left\{ \frac{1}{2} \frac{Z_g Z_{g'}}{r_{g g'}} - 2 Z_{g'} (g g' g) + 2 (g g' g g') \right\} \tag{9 a}$$

$$E_2 = - e^2 \sum_g \sum_{g'}{}^{(g)} (g g' g' g) \tag{9 b}$$

$$E_3 = e^2 \sum_g \sum_{g'} p_{g g'} \sum_{g''}{}^{(g)} \{ 2 Z_{g''} (g' g'' g) - 4 (g' g'' g g'') + 2 (g' g'' g'' g) \} \tag{9 c}$$

$$E_4 = e^2 \sum_g \sum_{g'} \sum_{g''} \sum_{g'''} p_{g g''}\, p_{g' g'''} \{ 2 (g'' g''' g g') - (g'' g''' g' g) \} \cdot \tag{9 d}$$

The symbols appearing here are defined by

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[1] The expression for an arbitrary ionic crystal consisting of ions with complete electron shells is obtained from (9), (9 a, b, c, d) by replacing g by (g, n) where n is an index enumerating the electron orbitals of the ion g.

$$(g g' g'') = \int \psi_g^*(\boldsymbol{r}) \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{g'}|} \psi_{g''}(\boldsymbol{r})\, d\boldsymbol{r}$$

$$(g g' g'' g''') = \int \int \psi_g^*(\boldsymbol{r}_1)\, \psi_{g'}^*(\boldsymbol{r}_2) \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \psi_{g''}(\boldsymbol{r}_1)\, \psi_{g'''}(\boldsymbol{r}_2)\, d\boldsymbol{r}_1\, d\boldsymbol{r}_2 .$$

From these definitions it is evident that[1]

$$(g g' g'') = (g'' g' g)^*$$

and

$$(g g' g'' g''') = (g' g g''' g'') = (g'' g''' g g')^* = (g''' g'' g' g)^*.$$

In order to make full use of (9), (9 a, b, c, d) we find it natural to consider the matrix $\boldsymbol{p}$ as a primary quantity, the calculation of which forms the first step in the solution of the problem.

If the condition[2]

$$\sum_{g'} |s_{g g'}| < 1 \tag{10}$$

is fulfilled for all g, the matrix $\boldsymbol{p}$ can be expanded in the power series[3] thus,

$$\boldsymbol{p} = \frac{\boldsymbol{s}}{1 + \boldsymbol{s}} = \boldsymbol{s} - \boldsymbol{s}^2 + \boldsymbol{s}^3 - + \tag{11}$$

The corresponding expansion $\boldsymbol{P} = \boldsymbol{S} - \boldsymbol{S}^2 + \boldsymbol{S}^3 - + \cdots$ mentioned in the introduction was introduced by Löwdin directly in (3 c, d). We have performed some preliminary calculations on LiH and found that the series (11) is not convergent because of the large overlapping of the H^--ions. Therefore we have tried to calculate $\boldsymbol{p}$ by another method, which seems to be generally useful in calculations according to the Heitler-London method.

We write (6) in the following form:

$$\sum_{g'} (\delta_{g g'} + s_{g g'})\, p_{g' g''} = s_{g g''}. \tag{12}$$

This is a system of N^2 linear equations with N^2 unknown quantities $p_{g g'}$. (N is the number of ions in the crystal.) The matrices $\boldsymbol{s}$ and $\boldsymbol{p}$ are both symmetrical, i.e., $s_{g' g} = s_{g g'}$ and $p_{g' g} = p_{g g'}$. When g and g' denote ions lying in the interior of a large crystal, the quantities $p_{g g'}$ must also have symmetry properties corresponding to the lattice symmetry. This is evidently true if the perturbation from the surface layer of the crystal can be neglected, which ought to be the case if the crystal is sufficiently large. (Throughout this paper we are disregarding the influence of surface effects.) The coefficients $\delta_{g g'} + s_{g g'}$ in

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[1] Evidently these relations remain true if the g are again interpreted as in the preceding note.

[2] As we consider a crystal of finite size, the matrix $\boldsymbol{s}$ is also finite.

[3] After we had arrived at the sufficient condition (10) for the validity of (11), Dr. Löwdin noticed and kindly pointed out to us that it can be found in Courant-Hilbert, Math. Physik I, p. 16.

(12) tend rapidly towards zero with increasing $r_{gg'}$, and it seems probable that the same is also true for $p_{gg'}$. After these arguments it seems promising to reduce the equation system (12) by making use of all symmetry properties of $\boldsymbol{s}$ and $\boldsymbol{p}$. This reduced system can then be approximated by taking into account only quantities associated with a few adjacent ions, whereby the number of resulting equations can be made rather small. We have tried this method and found it quite useful. The numerical calculations were carried out with the number of resulting equations ranging from 3 to 11. We found a satisfying convergence of the calculated matrix $\boldsymbol{p}$ with increasing number of equations. Further, the numerical results indicated that $p_{gg'}$ tends towards zero approximately as rapidly as $s_{gg'}$ with increasing $r_{gg'}$.

As previous authors have done, we shall separate E_{coh} (9) into elementary parts, going, however, into more detail (especially as regards E_4) and making no neglections. E_1 (9 a) can be written

$$E_1 = \frac{e^2}{2} \sum_{g} \sum_{g'}{}^{(g)} \left\{ \frac{\varepsilon_g \, \varepsilon_{g'}}{r_{gg'}} + \varepsilon_g \frac{\omega_{g'}(r_{gg'})}{r_{gg'}} + Z_{g'} \frac{\omega_g(r_{gg})}{r_{gg'}} - 2 (g' g g')_\omega \right\}, \tag{9 a$'$}$$

where $\varepsilon_g = Z_g - N_g$ is the valency of the ion g, and $\omega_g(r)$ is defined by[1]

$$\omega_g(r) = 8\pi \left\{ \int_r^\infty |\psi_g(x)|^2 x^2 \, dx - r \int_r^\infty |\psi_g(x)|^2 x \, dx \right\}.$$

This function is rapidly decreasing towards zero with increasing r. The new symbol in (9 a$'$) is defined by

$$(g g' g'')_\omega = \int \psi_g^*(\boldsymbol{r}) \frac{\omega_{g'}(|\boldsymbol{r} - \boldsymbol{r}_{g'}|)}{|\boldsymbol{r} - \boldsymbol{r}_{g'}|} \psi_{g''}(\boldsymbol{r}) \, d\boldsymbol{r}.$$

For E_2 we keep the formula (9 b), whereas E_3 (9 c) is transformed to the following form:

$$\begin{aligned} E_3 = e^2 \sum_{g} \sum_{g'}{}^{(g)} p_{gg} \left\{ N_g \frac{\varepsilon_{g'}}{r_{gg'}} - \varepsilon_{g'} \frac{\omega_g(r_{gg'})}{r_{gg'}} + 2 (g g' g)_\omega + 2 (g g' g' g) \right\} + \\ + 2 e^2 \sum_{g} \sum_{g'}{}^{(g)} \sum_{g''}{}^{(g)} p_{gg'} \left\{ \varepsilon_{g''} (g' g'' g) + (g' g'' g)_\omega + (g' g'' g'' g) \right\}. \end{aligned} \tag{9 c$'$}$$

E_1 (9 a$'$), E_2 (9 b) and E_3 (9 c$'$) are now written in such forms that every single sum in them is proportional to the crystal volume (if the lattice constant is kept fixed).

The corresponding transformation of E_4 (9 d) is more complicated, and therefore a special investigation is motivated. We begin by considering the following parts of the sum $2 e^2 \sum_{g} \sum_{g'} \sum_{g''} \sum_{g'''} p_{gg''} \, p_{g'g'''} (g'' g''' g g')$:

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[1] For crystals other than LiH this definition of $\omega_g(r)$ must be slightly generalized.

1°. The double sum D_1 that is obtained when $g' \neq g$, $g'' = g$ and $g''' = g'$. To estimate it we note that for large distances $r_{gg'}$ we have

$$(g g' g g') \sim \frac{1}{r_{gg'}}.$$

Hence

$$D_1 = 2\,e^2 \sum_g \sum_{g'}{}^{(g)} p_{gg}\, p_{g'g'}\, (g g' g g') \sim 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \frac{p_{gg}\, p_{g'g'}}{r_{gg'}}.$$

2°. The triple sum D_2 that is obtained when $g' \neq g$, $g'' = g$ and $g''' \neq \begin{cases} g \\ g' \end{cases}$. To estimate it we use (6) and get (for large distances $r_{gg'}$)[1]

$$\sum_{g'''}{}^{(gg')} p_{g'g'''}\,(g g''' g g') \sim \sum_{g'''}{}^{(gg')} p_{g'g'''} \frac{s_{g'''g'}}{r_{gg'}} = \frac{(\boldsymbol{p}\,\boldsymbol{s})_{g'g'} - p_{g'g}\, s_{gg'}}{r_{gg'}} =$$

$$= \frac{(\boldsymbol{s} - \boldsymbol{p})_{g'g'} - p_{g'g}\, s_{gg'}}{r_{gg'}} = -\frac{p_{g'g'} + p_{g'g}\, s_{gg'}}{r_{gg'}} \sim -\frac{p_{g'g'}}{r_{gg'}}.$$

Hence

$$D_2 = 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \sum_{g''}{}^{(gg')} p_{gg}\, p_{g'g'''}\,(g g''' g g') \sim -2\,e^2 \sum_g \sum_{g'}{}^{(g)} \frac{p_{gg}\, p_{g'g'}}{r_{gg'}}.$$

3°. The triple sum D_3 that is obtained when $g' \neq g$, $g'' \neq \begin{cases} g \\ g' \end{cases}$, and $g''' = g'$. By similar estimations as in 2° we get

$$D_3 = 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \sum_{g''}{}^{(gg')} p_{gg''}\, p_{g'g'}\,(g'' g' g g') \sim -2\,e^2 \sum_g \sum_{g}{}^{(g)} \frac{p_{gg}\, p_{g'g'}}{r_{gg'}}.$$

4°. The quadruple sum D_4 that is obtained when all four summation indices g, g', g'', g''' are restricted to be different from one another. By using similar estimations as before, we get

$$D_4 = 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \sum_{g''}{}^{(gg')} \sum_{g'''}{}^{(gg'g'')} p_{gg''}\, p_{g'g'''}\,(g'' g''' g g') \sim 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \frac{p_{gg}\, p_{g'g'}}{r_{gg'}}.$$

The above estimations of D_1, D_2, D_3 and D_4 can be made more exact, but for the sake of brevity we omit the calculations required. For a discussion of the D_i, we make the following remarks: It can be shown that, for fixed lattice constant, the sum

$$\frac{1}{V} \sum_g \sum_{g'}{}^{(g)} \frac{p_{gg}\, p_{g'g'}}{r_{gg'}} \tag{13}$$

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[1] The symbol $\sum_{g''}^{(gg')}$ means a summation over all g'' except $g'' = g$ and $g'' = g'$. The extension of this notation to the case when there are more restrictions is immediate.

tends to $+\infty$ with increasing crystal volume V, unless the condition[1]

$$p_{\mathrm{Li\,Li}} + p_{\mathrm{H\,H}} = 0 \tag{14}$$

is satisfied. If, on the other hand, (14) is satisfied, (13) is a sum of the Madelung type and has a finite limiting value. Our numerical calculation of the matrix $\boldsymbol{p}$ showed that (14) is not even approximately fulfilled (for LiH). Hence each one of the quantities $\frac{D_1}{V}, \frac{D_2}{V}, \frac{D_3}{V}, \frac{D_4}{V}$ tends towards $+\infty$ or $-\infty$ with increasing crystal size. However, their sum $\frac{E_4'}{V} = \frac{D_1 + D_2 + D_3 + D_4}{V}$ tends to a finite limit when $V \to \infty$.

It is convenient to write the sum $E_4' = D_1 + D_2 + D_3 + D_4$ as follows:

$$\begin{aligned} E_4' = {} & 2\,e^2 \sum_g \sum_{g'}{}^{(g)} p_{gg}\, p_{g'g'} \left\{ (g\,g'\,g\,g') - \frac{1}{r_{gg'}} \right\} + \\ & + 4\,e^2 \sum_g \sum_{g'}{}^{(g)} p_{gg} \left\{ \sum_{g''}{}^{(gg')} p_{g'g''}\,(g\,g''\,g\,g') + \frac{p_{g'g'}}{r_{gg'}} \right\} + \\ & + 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \left\{ \sum_{g''}{}^{(gg')} \sum_{g'''}{}^{(gg'g'')} p_{gg''}\, p_{g'g'''}\,(g''\,g'''\,g\,g') - \frac{p_{gg}\, p_{g'g'}}{r_{gg'}} \right\}. \end{aligned} \tag{9 d'}$$

The rest of E_4 (9 d) can be written[2]

$$\begin{aligned} E_4'' = E_4 - E_4' = {} & e^2 \sum_g p_{gg}^2\,(g\,g\,g\,g) + e^2 \sum_g \sum_{g'}{}^{(g)} \{ 4\, p_{gg}\, p_{gg'}\,(g\,g\,g\,g') + \\ & + p_{gg'}^2\,[3\,(g\,g'\,g'\,g) - (g\,g'\,g\,g')] - p_{gg}\, p_{g'g'}\,(g\,g'\,g'\,g) \} + \\ & + 2\,e^2 \sum_g \sum_{g'}{}^{(g)} \sum_{g''}{}^{(gg')} \{ p_{gg'}\, p_{gg''}\,[3\,(g\,g'\,g''\,g) - (g\,g'\,g\,g'')] - \\ & - p_{gg}\, p_{g'g''}\,(g\,g'\,g''\,g) \} - e^2 \sum_g \sum_{g'}{}^{(g)} \sum_{g''}{}^{(gg')} \sum_{g'''}{}^{(gg'g'')} p_{gg''}\, p_{g'g'''}\,(g''\,g'''\,g'\,g). \end{aligned} \tag{9 d''}$$

The right-hand sides of (9 d$'$) and (9 d$''$) are now written so that every single sum in them is proportional to the size of the crystal.

Previous authors[3] have classified the quantities according to their order of magnitude, essentially in the "overlap" of the atomic wave functions, and have neglected those of orders higher than an established one. This investigation shows, however, that only the complete expression for the cohesive energy has a real physical meaning and that great caution must be exercised in dividing it into partial sums. Because of the agreement between the calculated and the measured value of the cohesive energy for the crystals treated by Landshoff and Löwdin it seems probable that the terms they neglected are relatively small. For LiH the extension of the H^--ions complicates the problem, and a new investigation of this crystal, formerly treated by Hylleraas, has been undertaken. The numerical results will be published later.

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[1] In the interior of a large LiH crystal the value of p_{gg} depends only on whether g is a Li^+- or a H^--ion. In the former case the value is denoted by $p_{\mathrm{Li\,Li}}$ and in the latter by $p_{\mathrm{H\,H}}$.

[2] The expression (9 d$''$) has been simplified by observing that the Li^+- and H^--wave functions ψ_g are real.

[3] See p. 431, footnotes 1—3.

Lastly we will make a remark about Hylleraas' method of subtracting the energy of the free ions. If this energy is calculated by using the Hartree-Fock one-electron wave functions, which neglect "correlation", we introduce an error which can not be neglected when compared with the quantum mechanical part of the cohesive energy (i. e., the cohesive energy with the Madelung part disregarded). We have verified this assertion only for LiH, but it ought to be general. Using the subtraction method of Hylleraas, we might expect that the energy error for the crystal and the energy error for the free ions cancel each other to a large degree.

We wish to express our gratitude to Professor I. WALLER for suggesting to us a detailed quantum mechanical investigation of LiH, the origin of the present paper, as well as for his continued interest in our work. We are also indebted to Dr. P. O. LÖWDIN for many interesting discussions. Finally we wish to thank Dr. Phil. P. KUHN for help with some preliminary calculations.

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